# How to provide an equilibrium to the optimizers, and a review of 3D MHD and related topics

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This document has three parts. First, a chronological list of publications relevant to the study of three-dimensional (3D), magnetohydrodynamic (MHD) equilibrium theory and computation, coil design, etc. is assembled. Second, an "action plan" for how to proceed with the equilibrium calculation for the Simons proposal is described. Third, a comprehensive, meandering discussion of anything and everything that might be relevant is *under construction*.

**CRITICISMS, SUGGESTIONS AND QUESTIONS ARE SINCERELY WELCOME AND ENCOURAGED**

I am of course most familiar with my own work, so please forgive me if the following is biased; and a small set of the "good ideas" on how to proceed originated with me. The more that everyone contributes, and the more that this draft proposal reflects the summation of our knowledge, intelligence and imagination, the more likely that our proposal, fusion energy and humanity will be successful. Please contribute text, references, figures etc.

**Contents**

# I. PUBLICATIONS

The following publications create a chronological list of papers in the bibliography. Well, it with with `bibliographystyle{unsrt}` with less than 256 references??? Now I am using `\bibliographystyle{alpha}`. Can anyone help me prepare a chronological list with unlimited citations?

These papers have, in some fashion, contributed to the understanding of three-dimensional MHD equilibria.

Please inform me of any papers that are missing, and I expect that there are many. For each paper, you are welcome to provide a couple of sentences that briefly describe the contribution presented therein; and to provide any figures that may be suitable.

## A. chronological list of publications

1954 [Kol54]
1955
1956 [Niv56]
1957 [CK13]
1958 [Wol58] [Wol89] [GR58] [BFKK23] [KK84] [Spi83]
1959
1960
1961
1962 [Mos62]
1963 [Arn63]
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1965
1966 [RSTZ66]
1967 [Gra65]
1968
1969
1970
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1972 [SZ72]
1973 [RDR73]
1974 [Tay74]
1975 [BG75]
1976
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1978 [BBG78]
1979 [Gre79] [Chi79] [Per79a] [Per79b]
1980 [PMWJ80] [Rei80]
1981 [Boo81] [CS81] [Rei81]
1982 [BBG82] [BG82] [Car82] [BD82] [Boo82] [Mat82]
1983 [CL83] [Boo83] [Aub83] [Kar83] [MM83] [ALD83] [BW83] [HW83] [Mac83]
1984 [BBG84] [BWD 8] [BF84] [She84] [Boo84] [RB84] [MMP84b] [Car84] [MMP84a] [HC84]
1985 [HCGR85] [HM85] [FA85] [CK85]
1986 [Tay86] [CH86] [HL86] [HH86] [PMSM86] [GMS86] [BFL+86] [Mat86] [Mer86] [HvRM86] [RG86]
1987 [Fre87] [MMP87] [Merdf]
1988 [Bet88] [LHHN88] [RG88]
1989 [RPB89] [HB89] [GRS89] [HHS89] [Rom89] [MS 8] [Mac 0]
1990 [NWHB90] [MD90] [HST90] [RG90] [HSN90] [RKW90]
1991 [GB91] [CH91] [HBNW91] [DHCS91] [RP91] [HB91] [RKW91]
1992 [CHMG92] [GLM+81] [LH92] [MS92a] [DM92] [Mac92] [Gol92] [Coo92] [WR92] [Coo92] [MS92b] [GB92] [Mei92]
1993 [MC93] [Sch93] [Tay94] [MM93]
1994 [BER94] [Mei94] [KB94] [Par94] [HSM+94] [Mei94] [Han94] [DHP94] [KS94] [LS94] [Kai94] [SL94] [LS94]
1995 [Fit95] [BHH+95] [BL96]
1996 [Gar96] [HD96]
1997 [GLHH97] [ECVD97] [HD97a] [HD97b] [DH98] [SHW97]
1998 [MCG+98] [HD98] [HB98] [Gar98] [LGHH98] [HWB+98]
1999 [Boo99] [PBF+99] [HD99] [Ber99]
2000 [LFLM00] [Heg00] [SHWW00] [FKC+00] [NRZ+00] [ZBB+00] [SPS+01]

2001 [SLK01] [RKM+01] [IWU+01] [ZBB+01] [SHB+01] [SLK01] [HMR01]
2002 [HMK+02] [Gar02] [HMR+02]
2003 [NB03] [Spi03] [SGH+03] [Spo16]
2004 [CBC+04] [SGG+04] [EL04] [KU04] [Hud04] [EMT+04] [KU04]
2005 [DMR05] [SNW+06] [Spo72]
2006 [ORM06] [Hud06] [HHD06] [BN06] [Mac 0]
2007 [RZM+07] [PBB+07] [JBF07] [PBG07] [Hud07] [HHD07a] [HHD07b]
2008 [HB08] [DHM+08] [EGWH+08] [LMP+09] [PM08]
2009 [Hud62] [CB09] [MHD09] [HMHD09] [GM09] [HD09] [NBH09] [HHK+09] [KR09]
2010 [BCC10] [BP10] [HN10] [CGP+10] [GM10] [Hud10] [MHDvN10] [SBB+10] [Spo10] [SH39]
2011 [Heg11] [HSC11] [IC11] [Bar11] [SH12] [FC11]
2012 [SHS+12] [DHG12] [LLH+12] [Heg12] [Laz12] [HDD+12] [QLLS12, CF13, QLLS13]
2013 [SHS+13] [DHDH13] [DHG13] [LC13] [DHT+13] [HN13]
2014 [DHDH14b] [HS90] [HSF44] [DHDH14a] [Wei14] [Cla12]
2015 [LHBH15] [KSL+17] [Mof15] [DYBH15] [RFT+26] [LHB+15] [Zak15] [BBG+15] [Han15] [Spo55]
2016 [LHN16] [LLHH16] [Rei00] [LB16] [FM16] [Wei16] [LLHH16] [Esc16] [LAH16]
2017 [LH17a] [KH17] [HK17] [PRRBS+17] [GBB+a0] [Land4] [ZHSW0a] [Suzdc] [KAS+18] [SHTO01] [VSG04] [VSGc4]
2018 [HLL18] [ZHSW18] [ZHL+18]

## II. PLAN OF ACTION FOR 3D EQUILIBRIUM

### A. vacuum fields

Let's start with the simplest MHD equilibria possible, that of vacuum fields. There is a fantastic amount that we study. Vacuum fields are particularly attractive because we have exact, well-defined solutions.

There are two ways to compute vacuum fields, either via solving Laplace's equation or via solving the Biot-Savart law.

#### 1. *Laplace solvers*

1. Develop a fast three-dimensional (3D) Laplace solver: given a closed toroidal boundary, $\partial\mathcal{V}$, which encloses a volume, $\mathcal{V}$, and the boundary condition, e.g. $\mathbf{B}\cdot\mathbf{n}$ on $\partial\mathcal{V}$, and a loop integral, $\int \mathbf{A}\cdot d\mathbf{l}$, to constrain the toroidal flux, the vacuum field inside the boundary is unique. Cerfon *et al.* are developing fast integral solvers that have many advantages, not least of which is that a coordinate grid is not required in the $\mathcal{V}$, only $\partial\mathcal{V}$, needs to be discretized.

#### 2. *Biot-Savart solvers*

Eventually, we need current-carrying coils to provide the magnetic field. Traditional approaches introduce a current potential on a arbitrarily defined winding surface, which is then discretized to obtain a discrete set of coils. A recent approach starts with a representation of the discrete set of coils directly. (See Sec. VII B.)

1. Develop a fast Biot-Savart solver: given the geometry of a set of coils, determine the magnetic field at an arbitrary point. To begin, for simplicity, we can assume the coils are zero-thick, but ultimately we need to consider finite-thickness coils. Whenever the plasma is close to the coils (as in LHD), the finite-thickness of the coils becomes important.

#### 3. *vacuum field optimization*

Is is true to say that at least some plasma properties, if not many, do *not* depend on the MHD equilibrium itself, but only depend on the magnetic field? We can investigate every such property in vacuum fields. By this I mean that we can test ideas, algorithms etc. (The vacuum field is completely stable, so of course we cannot study instabilities in vacuum.)

The Optimizers can consider the following.

1. Introduce a measure of "coil complexity", $\mathcal{C}$, that reflects engineering difficulty, cost, etc. of a given coil set. How does the coil complexity vary with each of the considerations listed below?

2. An analysis of which normal field distributions on a given winding surface can be "efficiently" produced may fantastically reduce the search space for the coil geometry. (See Sec. VII B, and Boozer/Landremann can elaborate on this point.) Rather than considering all possible vacuum fields, we can restrict attention to those which can produced with easy-to-build coils.

3. How integrable can a field without a continuous symmetry be? The need for integrability is described in Sec. VI A. A brief review of some theorems and results, algorithms for improving integrability etc. in chaos and non-linear dynamics is provided in Sec. V; and many of these ideas have already been applied to magnetic fieldline flows, see Sec. V B and Sec. V C. *Robert MacKay: Id expect it cant be perfectly integrable, but dont know how to prove it. And maybe Im wrong and there are some superb examples, like the magic integrable systems such as Jacobi geodesics on an ellipsoid or Calogero-Moser or KdV. When we allow plasma and dont require Beltrami then do we get integrable B? cf. incompressible fluids where either Bernoulli const provides integrability or v parallel to vorticity with nontrivial variation of the factor provides integrability.*

4. The rotational-transform measures how many times on average a fieldline wraps around the torus poloidally per toroidal transit, $\iota\!\!\!-\equiv \Delta\theta/\Delta\zeta$. The need for rotational-transform is described in Sec. VI B, and vacuum fields *must* have 3D shaping to produce rotational-transform. How much rotational-transform can be produced by 3D shaping? Should we dial in the preferred finite-pressure rotational-transform into the vacuum field, or should we let the self-consistent plasma currents do the work?

5. Do we need to constrain in detail the entire rotational-transform, $\iota\!\!\!-(\psi)$, as a function of enclosed toroidal flux? Can we make progress by only considering the rotational-transform on axis and the edge? Can perfectly flat rotational-transform profiles be constructed? (Such profiles will avoid the problems with resonances at rational-surfaces.) Thinking ahead to finite-pressure plasmas, the rotational-transform profile has an important effect on instabilities.

6. Are the requirements of integrability consistent with high rotational-transform? Or, perhaps integrability is more closely related to shear, which describes how the rotational-transform varies with minor radius. Before we imagine to achieve challenging goals, such as simultaneous achievement of {integrability} + {high rotational-transform} + {quasi-symmetry}, we need to ensure that we can achieve the simpler goals, such as just {integrability} + {high rotational-transform}.

7. How much quasi-symmetry can be produced? Is quasi-symmetry consistent with integrability and high rotational-transform? Perfectly integrable, perfectly quasi-symmetric can easily be produced in axisymmetric geometry. Consider the constrained functional

$$\mathcal{G} \equiv \omega_1 \mathcal{Q}^2 + \omega_2 \mathcal{I}^2 + \lambda(\iota\!\!\!- - \iota\!\!\!-_0), \tag{1}$$

   where $\mathcal{Q}$ and $\mathcal{I}$ are measures of quasisymmetry and integrability that we wish to minimize, $\omega_i$ are weights, and $\lambda$ is a Lagrange multiplier. Extremizing $\mathcal{F}$ finds a field with constrained rotational-transform, $\iota\!\!\!- = \iota\!\!\!-_0$, where $\iota\!\!\!-_0$ might be the rotational-transform on axis. We can find a sequence of fields with increasing rotational-transform by varying $\iota\!\!\!-_0$, and we can determine how quasisymmetry and integrability degrade.

8. We can test, in vacuum fields, all of our understanding, and "guesses", and numerical routines for diagnosing the structure of chaos; such as: finding the magnetic axis; finding the size of magnetic islands; straight fieldline coordinates; cantori; turnstiles, the last closed flux surface (boundary surface); computing Lyapunov exponents; volumes of ergodic regions; transport of magnetic fieldlines; and all properties regarding the structure of magnetic fields that we deem important.

9. Single particle trajectories may be examined, either using the guiding center approximation or using the full-particle motion if required. Do high-energy $\alpha$-particles produced by fusion reactions (remember that we are trying to create fusion) require a special treatment? For which type of particles should we optimize the properties of the vacuum field? Single-particle motion is described by the single-particle Hamiltonian. How do single particles traverse across the last closed flux surface, across the stochastic edge and collide with the vacuum chamber? How do islands of single particle trajectories correlate with magnetic islands of the field? How do cantori of single particle trajectories correlate with cantori of the magnetic fieldlines?

10. How does heat and density traverse from the core the the wall? *Robert MacKay: this is something Im keen to contribute to. I think the standard approach to cross-field transport from two-body interactions is inadequate. My paper with Pinheiro [PM08] shows what really happens in a uniform magnetic field. Needs adapting to a curved one.*

11. Are computationally intensive calculations necessary, or can turnstiles, cantori, ghost surfaces/chaotic coordinates etc. provide a simple accurate description of transport across the edge?

In addition to the above topics that characterize the properties of magnetic fields, we can ask the following questions about the coil geometry.

1. Each "coil set" generally includes modular coils, helical coils, trim coils, vertical field coils. What is the optimal "linking arrangement" for a given desired vacuum boundary?

2. How does the complexity, $\mathcal{C} = \mathcal{C}(\mathcal{I}, \iota\!\!\!-, \mathcal{Q})$, of the coils depend on integrability, transform and quasisymmetry? This function can be determined numerically, and therefore it is quite likely possible to determine analytical expressions.

3. How do coil placement errors affect the vacuum field? How precisely do the coils need to be built? This has a direct impact on cost. What is the relationship between integrability, transport across the chaotic layer, rotational-transform to coil-placement errors?

4. There is theoretical and numerical evidence of "self-healing", where the size of vacuum magnetic islands reduces with increasing plasma pressure. Should the vacuum state be designed with such islands, so that the high-pressure equilibrium is healed? Magnetic confinement of plasmas is such a complicated issue (very worthy of Simons) that not even the required vacuum fields can be identified without an understanding of plasma effects.

5. Introduce a measure of "flexibility", $\mathcal{F}$, of the coil set that measures how many different magnetic fields can be produced by a given coil set by only varying the coil currents? See Sec. VII D 2. Imagine we have a set of coils, $\mathbf{x}_i$, each carrying current $I_i$. How do integrability, rotational-transform, quasisymmetry etc. all depend on $I_i$. Can the island content of a vacuum field be varied, without changing the "average" rotational transform, just by varying the currents in the modular coils? What is the optimal design of trim coils for fine-tuning islands, structure of the ergodic edge?

The only impact of the MHD equilibrium itself on properties that depend only on the magnetic field is to change the magnetic field, $\mathbf{B}_T = \mathbf{B}_C + \mathbf{B}_P$, where $\mathbf{B}_T$ is the total magnetic field, $\mathbf{B}_C$ is the "vacuum" magnetic field produced by external current-carrying coils, and $\mathbf{B}_P$ is the magnetic field produced by plasma currents.

We should begin with optimizing every conceivable property of vacuum fields, which should include a consideration of the coil geometry and cost. We should also understand which properties of vacuum fields are consistent with each other and which are not. If we cannot get our all of our calculations working for vacuum fields, then ***Do Not Pass Go. Do Not Collect $3,000k***.

Vacuum fields present an *exact* challenge for the numericists because the fields are known exactly, but they are also immediately relevant to experiments. Experimentalists must have a "startup scenario", see Sec. VII D 3.

## B. On 3D MHD equilibria

Vacuum fields are easy: zero pressure, zero current, continuous and differentiable magnetic fields and no assumptions on the topology of the field. Plasmas are a much more difficult proposition.

Equilibrium codes make assumptions about the structure of the pressure profile: whether it is smooth, continuous, or discontinuous. Equilibrium codes also, *by definition*, make assumptions about the topology of the magnetic field, so that the magnetic field is consistent with an assumed pressure profile; see Sec. IV B. One might say, because of the topological assumptions, that there is a "theoretical discontinuity" between vacuum fields and equilibrium fields; and this is why initial value codes Sec. IV C, which do not require topological assumptions, will always be intriguing. This subsection will persist with the equilibrium approach.

To get to a stellarator, we must be both practical when we have to be and rigorous when we can be.

### 1. *analogy with the aerospace*

Perhaps a suitable analogy can be made with the aerospace industry. After a *lot* of trial-and-error, in 1903 the Wright brothers first got a flying contraption off the ground for a total time of 12 seconds! The pioneers in the field did not get every mathematical detail to machine precision (there was not even a concept of machine precision, as computers were not yet invented), but they made guesses and approximations. It was 66 years later that a human took a small step on the moon. By this measure, progress towards fusion is well on track!

We must also acknowledge that stellarator research has made fantastic progress, and we may argue that the experiments (which were designed using existing algorithms) have already confirmed that well-defined solutions to well-defined mathematical equations must exist. We, the mathematicians, just need to find out what these equations and solutions are.

### 2. *practical versus rigorous*

The following outline shall mix practical considerations, which primarily includes everything warts-and-all that is already working, with an attempt to identify areas which either demand a more mathematically rigorous approach, those for which a more rigorous approach is preferred, and those areas for which a systematic investigation might be used to show why a less-than-rigorous method that seems to work is trustworthy.

## C. equilibria with nested surfaces (VMEC and NSTAB)

In parallel to the above investigations of vacuum fields, we must start with the most widely used MHD equilibrium code. VMEC output is used as input for linear stability codes, transport codes, etc. The main flaw of VMEC is the inaccurate treatment of singular currents, see Sec. III K, at rational surfaces and/or the formation of magnetic islands. We can only go as far with VMEC as we are confident that VMEC is getting a sufficiently accurate equilibrium. We either need a measure of the island content that *should* be present in a given VMEC equilibrium.

1. Linearized calculations, see Sec. III W, that take an approximate (i.e., VMEC) equilibrium and compute the first-order correction to bring the equilibrium closer to a "perfect" equilibrium have been developed. These

conceivably provide a measure of the "island content" in VMEC, which must be reduced by the optimization. These measures can be tested on vacuum fields. Whether this is a practical approach needs to be confirmed, but it is likely *not* a rigorous approach, as ideal-MHD are not analytic [RDR73].

2. NSTAB is quite likely a more accurate equilibrium solver than VMEC, and it is precisely because of this that NSTAB is more fragile and is not as widely used as VMEC, see Sec. III F. NSTAB employs a conservative discretization that recognizes islands as sheet currents. Recently a model of ideal-MHD with continuously nested surfaces and with sheet currents has been rigorously formulated and this model suggests that ideal MHD equilibria with nested surfaces must have sheet currents that cause discontinuous rotational-transform, see Sec. III S. A very interesting effort would be to re-build VMEC and NSTAB to officially allow sheet currents, and/or to determine if the first-order correction described in the above list item *can* be made rigorous by allowing for discontinuous transform. The optimizer would then seek equilibria for which the sheet currents = islands are minimized.

3. There is some evidence that VMEC is performing satisfactorily well when compared to experimental results, see Sec. III L, and this is perhaps the only important concern. Take a plasma property, $\mathcal{P}(\mathbf{B})$, of interest, expressed here as a function of the equilibrium magnetic field, $\mathbf{B}$. Imagine that the "true" equilibrium magnetic field for a given boundary and a given set of assumptions is given by $\mathbf{B}_T$, and that the "numerical" equilibrium computed by VMEC, or any code, is given by $\mathbf{B}_V$, and the error is $\delta\mathbf{B} \equiv \mathbf{B}_T - \mathbf{B}_V$. The question of practical concern is: what is
$$\delta\mathcal{P} \equiv \frac{\partial \mathcal{P}}{\partial \mathbf{B}} \cdot \delta\mathbf{B}? \tag{2}$$
Consider computing a measure of single-particle transport in a vacuum field, and the same measure of single-particle transport in the VMEC approximation to the same vacuum field. What is the difference? How does the difference change when there is an island in the vacuum? Do the measures of island width that may be extracted from VMEC/NSTAB allow the island width to be so effectively reduced (in a vacuum optimization based on VMEC/NSTAB) so that the single-particle transport in the true vacuum field is identical (or close enough) to the single-particle transport in the VMEC/NSTAB field?

4. The mathematical conditions required for an equilibrium consistent with nested flux surfaces has been investigated by Weitzner, see Sec. VI G. These predictions could be confirmed and perhaps "hardwired" into the equilibrium calculation. By doing so, is it possible to restrict attention to only equilibria with nested surfaces that are guaranteed to avoid non-physical singularities? This would greatly reduce the search space.

The above items are suggestions on how to test various ideas in vacuum fields. What comes next is low-pressure plasmas.

### D. very-low $\beta$ plasmas

The magnitude of the plasma pressure is very often normalized to the magnetic pressure,
$$\beta \equiv \frac{\int p\, dv}{\int B^2\, dv}. \tag{3}$$
A lot of early theory of stellarator theory was based on expanding from a vacuum field using low-$\beta$ as an expansion parameter, see Sec. VI E. These approaches conceivably will allow an extension of the rigorous verification exercises discussed above for quantifying how well our equilibrium models treat vacuum fields into finite-pressure plasmas.

1. Do the various equilibrium models based on VMEC and/or NSTAB described above in Sec. II C recover the analytic predictions in the low-$\beta$ limit? If not, why should we believe such equilibrium codes for high-$\beta$ plasmas?

2. Some of these predictions suggest that islands present in the vacuum state with "self-heal" as pressure is increased; see Sec. VI E. Should we therefore pre-load islands into the vacuum state? If so, which islands, how large should they be and which phase?

### E. general finite-pressure plasmas

1. Do we need to only consider equilibria with nested flux surfaces if we can confident that that is what the Optimizers will find?

2. An alternative path for the equilibrium is to assume that the optimization algorithm will select only equilibria with a continuous foliation of nested flux surfaces, as most would expect that integrable magnetic fields provide better confinement. If we were to apriori restrict attention to such healed equilibria, then the equilibrium approach described in Sec. VI G might be the way to go. (Doing so however, will limit the equilibrium code applicability to real experimental configurations, which cannot be assumed to be perpetually healed; and it would certainly be desirable to have an equilibrium code that can be used outside of configuration optimization studies.)

3. To go beyond optimizations based on VMEC, one path is to pursue numerical development of the mixed ideal-relaxation equilibrium model described in Sec. III T and in Ref. [HK17], which will employ algorithms from VMEC and SPEC. This model presents a *continuous* generalization of ideal MHD and Taylor relaxation and allows for relaxation (and islands, chaos) at the rational surfaces, smooth pressure profiles and continuous magnetic fields. (The other two well-defined equilibrium models, namely stepped pressure and stepped transform, both require tangential discontinuities in the magnetic field.) Such a model could become very fast, particularly when using the fast Beltrami solvers being developed by Cerfon *et al.* . The ideal relaxed model is both an analytic function of the boundary and provides a less-ambiguous measure of the island size.

4. We may even consider an almost-fractal, smoothed devils staircase equilibrium . . .

5. Linear stability should be easy to compute, at least conceptually. Given an energy principle, setting the first variation to zero defines an equilibrium state, and then computing the "sign" of the second derivative (i.e., by performing an eigenvalue analysis of the Hessian) determines linear stability. The same constraints on the topology, helicity that were imposed to calculate the equilibrium state should also be imposed when calculating the eigenvalues. The linear stability calculation will thus allow for mix of flux surface and islands.

### F. linear stability versus nonlinear stability

Historically, the linear stability of the equilibrium state was of paramount concern. For example, that the plasma must be stable to so-called "high-$n$" interchange modes was a "given", and stellarator optimization calculations imposed the constraint of Mercier stability (i.e., that there was a magnetic well). For tokamaks, in which the confining magnetic field is partly produced by plasma currents, a linear instability can easily trigger a global instability. For stellarators, in contrast, the confining magnetic field is primarily produced externally; and there is very little that the plasma can do to break the magnetic bottle. This conjecture is supported by experimental observations.

If this is indeed so, it is a fundamentally important concern. We can relax the constraint that plasmas need to be linearly stable, provided that they are of course nonlinearly stable. This could greatly enhance our freedom to find optimal equilibria.

An equilibrium state is a *minimum* of the energy functional subject to imposed constraints on the plasma motion; elsewhere in this document we have considered what the appropriate constraints are. Such a state, by definition, is linearly and nonlinearly stable. If the plasma is perturbed, then it may wobble and thrash around, but it cannot degrade the magnetic bottle, and it cannot escape. But, for a numerically calculated minimum energy state, this is only guaranteed for a restricted class of variations, namely those resolved by the numerical resolution.

We also need to consider the importance or otherwise of high-frequency plasma oscillations, i.e. "high-$n$" instabilities, which cannot usually be resolved in the equilibrium calculation. If it can be ensured that these are benign, the optimization problem becomes much simpler; but, there is much that needs to be confirmed.

1. Is linear stability, even for low-$n$, of the plasma important given that the equilibrium is a minimum energy state? Can energy principles be used to show under what conditions, if any, the plasma can break the magnetic bottle?

2. Are high-$n$ instabilities important? At sufficiently small scales, do non-MHD effects (such as the finite Larmor radius) damp and stabilize the oscillations?

3. Is there a large-scale instability that degrades plasma performance, i.e. degrades quasisymmetry?

4. Even if they do not lead to disruptions, it is expected that micro-instabilities will enhance particle transport, and thereby degrade confinement.

We may also consider instabilities that corrupt stellarator-symmetry and/or field periodicity, but these are a practical rather than fundamental concern. To study large-scale symmetry and periodicity breaking instabilities, we just need to allow for such variations in the equilibrium calculation.

### G. free-boundary calculations

This section is under-construction, see Sec. III Q for some background.

1. Free-boundary equilibrium codes must almost certainly be employed. The independent degrees of freedom in the optimization describe the coil geometry, and measures of coil complexity and plasma properties, including transport across the chaotic edge, can simultaneously be quantified.
2. In the relaxed regions, nested flux surfaces are not guaranteed, and magnetic coordinates cannot generally be constructed. Codes that compute transport will need to be developed that can accommodate non-integrable magnetic fields.

### H. including small, non-ideal terms

1. We can always imagine including additional physics into the equilibrium. Assuming $\nabla p = \mathbf{j} \times \mathbf{B} + \epsilon \mathbf{f}$, where $\mathbf{f}$ is a given "non equilibrium" additional force, from plasma flow for example, can we compute a self-consistent equilibrium using perturbation theory?
2. Instead of infinite parallel transport of pressure, a more realistic model is to assume an anisotropic model for which there is a strong parallel diffusion balanced by a small perpendicular diffusion, and to include small non-ideal terms into the equilibrium equations. The pressure profile becomes a *smoothed* devil's staircase [HB08, Hud62], and the pressure profile for a given magnetic field be solved analytically, even for non-integrable fields, using chaotic coordinates.

### I. resistive initial value codes

MHD equilibrium theory is the simplest possible model and more physically realistic models exist, see Sec. IV C. By including resistivity, the problems with non-integrable singular currents are removed and the apriori assumption of topological constraints are not required.

1. Imagine we obtain a desired equilibrium, and that we use this equilibrium to initialize a resistive initial value code, see Sec. IV C. Should the equilibrium remain generally intact? Resistive MHD codes (NIMROD, M3D-$C^1$) are slower than equilibrium, but perhaps these can be used as an aposteori reality check?
2. Given that the resistive MHD codes are slower, perhaps we can create equilibria that are particularly easy for these codes. That, can we construct some "dedicated equilibria" with very simple geometry for example, that will provide an opportunity for a rigorous verification calculation between the equilibrium codes and the resistive initial value codes as the resistivity approaches zero? The challenge will be that singularities inherent in ideal MHD will reappear as the resistivity vanishes, but if we can create equilibria that are self-consistent without singular currents, then there is an excellent opportunity for a rigorous verification.

### J. On closing the loop

The primary "output" of the equilibrium calculation is the magnetic field, and this depends on the assumed pressure, rotational-transform/current profiles, but the profiles depend on the transport, which depend on the equilibrium magnetic. We need to "close the loop".

1. Is this just to be left to the Optimizers: to compute the field, the transport, the pressure, and then to compute the field? Can we approximate the closing of the loop?

### K. stellarator symmetry

Can anyone provide a compelling reason of why stellarators are designed to be stellarator symmetric? It makes the codes faster, but what is the fusion advantage. Modern tokamaks are *not* stellarator-symmetric, even though they are axisymmetric. Stellarator symmetry is analogous to time-reversal symmetry [DH98], or up-down symmetry in axisymmetric geometry.

1. The various mathematical tools should accommodate non-stellarator-symmetric configurations unless a compelling reason is provided.

### L. why not knots?

Stellarators may also be built in the shape of knots, see Sec. VII A. No clear advantage to knotatrons has yet been put forward, but this is only because that the mathematical tools required to investigate the plasma properties cannot yet accommodate general *topological* toroidal geometries.

1. Unless a compelling reason why knotatrons cannot have advantages, the mathematical tools should allow arbitrary toroidal boundaries. This is quite simple actually: instead of restricting attention to toroidal surfaces parameterized by $\mathbf{x}(\theta, \phi)$, where $\theta$ is an arbitrary poloidal angle and $\phi$ is the cylindrical toroidal angle, the codes should simply use the general parameterization, namely $\mathbf{x}(\theta, \zeta)$ where both $\theta$ and $\zeta$ are arbitrary. This is the general representation for a two-dimensional surface embedded in three-dimensional space, and we could look at any knotted configuration. It is not just for knots that a generalized toroidal angle would useful: using $\phi$ is inefficient for the QP/QI configurations produced by Spong and Harris [SH39] (I can't download the figure; please provide the figure.)

2. Different knots allow different linking arrangements of the coils and the plasma. It is entirely plausible that a non-trivial knot may allow an as-yet-unimagined coil arrangement that provides advantages. We should explore and categorize the family of knotatrons and their coils from a topological/linking perspective.

### M. the "fixer-upper" approach: building flexible coils

Or we need a way to correct the islands no matter what.

1. Another more cavalier approach is to proceed without caution with e.g. VMEC, provided that we construct appropriate "trim coils" that can be used to control the size of magnetic islands in real time during the experiment. That is, it is certainly plausible that none of these equilibrium issues actually need to be addressed to perfect satisfaction. Instead, the real problem is to design a sufficiently flexible experiment, that can vary the rotational-transform profile about some preferred state, and that all relevant resonant fields can be controlled aposteori by trim coils. Simple?

2. Can an equilibrium state be constructed so that, not just are the plasma properties optimized, but that the sensitivity of the plasma properties to errors in the numerical equilibrium approximation, coil misplacement errors etc. are minimized?

### N. On stellarator optimization

1. What is it that we will do that has not already being done? If our task is to design a practical experiment, the paper by Gates *et al.* [GBB$^+$a0] should really be required reading and the starting point for our discussion.

## III. 3D MHD EQUILIBRIUM THEORY AND NUMERICS

There are various definitions on what constitutes a 3D MHD equilibrium code. One objective of this review is to place the different approaches into some context, and to suggest a common terminology.

Broadly, the structure of this document is as follows. First, approaches based on the energy principle are reviewed. Then, approaches that may be described as initial-value or iterative algorithms are described. Methods that do not fit neatly into these first two categories are mentioned thereafter.

Following that, and specifically to the Simons proposal, various questions and suggestions regarding how we should proceed from here are listed.

It is my hope that this document will eventually become a comprehensive, unpublished, community-authored review of research and promising avenues of future research into "how to design and build a stellarator".

### A. prelude: on numerical error

First and foremost, the recurring theme of *historical* 3D MHD equilibrium calculations is an expedient "interpretation" of numerical error. This must be forgiven, as well-defined mathematical models were not available until 1996 [BL96]; but, stellarators were already being built. To advance, the stellarator community embraced the best available numerical calculations of equilibria that were being realized experimentally.

From a strict mathematical sense, numerical error is well defined: it decreases reliably and predictably as the numerical resolution increases. This assumes that there is a well-defined solution to the equation at hand, and that the numerical discretization accommodates the structure of the true solution. If the "error" does not decrease as the resolution increases, it is not numerical errors that we should be concerned with: we should acknowledge that there is a "mistake" in either the theory, the numerics, or both.

Traditionally, however, a well-defined solution to 3D MHD was not at hand. Harold Grad [Gra65] is frequently quoted as "3D MHD equilibria are pathological". Concerns such as these were ignored because of the lack of preferable alternative; and to its credit the international stellarator community marched forward. Today we have W7-X.

It is the opinion of this review that many 3D MHD codes, perhaps understandably, *needed* "numerical error" to regularize and/or provide context to an otherwise imprecisely defined algorithm. Unfortunately, to understand how finite numerical resolution impacts a given algorithm one needs to understand not just the theory upon which the algorithm was based but also the numerical discretization. This invariably requires first-person experience running a given code, and perhaps a detailed reading of the source. This is more than unfortunate.

There is a large amount of work in the field of 3D equilibria that implicitly requires finite numerical "error" and/or adhoc numerical schemes to regularize unphysical, ill-posed or otherwise fragile algorithms. A pioneer in the field of 3D MHD equilibria, Paul Garabedian was an excellent mathematician but he was also very practical: "if a code converges, it works" [private communication]. Garabedian also provided a philosophical interpretation of the role played by numerical error [I will try to recover the paper by PG that mentioned this; Garabedian's bibliography is online [https://www.math.nyu.edu/faculty/garabedi/cvpg.pdf]]. Finite numerical resolution could be interpreted as a small-but-finite plasma resistivity; e.g., the numerical error $h^2 \sim \eta j^2$, where $h$ is the grid resolution, $\eta$ is the resistivity, and $j$ is the current-density. Any plasma resistivity regularizes the singularities inherent in ideal MHD.

However, as the numerical resolution increases, the artificial "plasma resistivity" vanishes, and the equilibria approach the pathological states described by Grad [Gra65]. No code has been yet developed that can truly handle the fractal "pathological" structure. Any code that requires "numerical error" produced by finite numerical resolution to be interpreted as being either physically meaningful or required to regularize mathematical singularities should be treated with suspicion.

Fortunately, we have made progress. Well-posed mathematical models of 3D MHD equilibria have now been discovered, and the stellarator community should support their numerical implementation: see the stepped pressure model of Bruno & Laurence, Sec. III O, multi-region relaxed MHD, Sec. III P; the stepped *transform* model of Loizu, Hudson *et al.*, Sec. III S; and the unification of the stepped pressure and stepped transform models in the mixed ideal-relaxed model that accommodates smooth pressure and continuous magnetic fields, Sec. III T.

### B. Vacuum fields

Vacuum fields can be solved using Laplace's equation . . .

### C. Energy Principle

In the beginning, back in 1958, Bernstein, Frieman, Kruskal & Kulsrud created the energy functional [BFKK23, KK84],

$$W \equiv \int_{\mathcal{V}} \left( \frac{p}{\gamma - 1} + \frac{B^2}{2} \right) dv, \tag{4}$$

where $\mathcal{V}$ is the plasma volume, $p$ is the plasma pressure, and $\mathbf{B}$ is the magnetic field. (The work was actually performed in 1954 but was only published when fusion was declassified [R. Kulsrud, private communication].) Equilibria are extrema of this functional.

If there are no constraints on the allowed variations, extrema satisfy $p = 0$ and $B = 0$, and the extremizing solutions are completely irrelevant for our purposes. So the question is: what are are the allowed variations of the pressure, $p$, and magnetic field, $\mathbf{B}$ that should be considered in extremizing the energy functional?

### D. ideal variations

So-called "ideal variations" are derived from the equation of state, $d_t(p/\rho^\gamma) = 0$, where $d_t \equiv \partial_t + \mathbf{v} \cdot \nabla$ and $\mathbf{v}$ is the "velocity" of an assumed plasma displacement, $\mathbf{v} = \partial_t \boldsymbol{\xi}$, which is combined with mass conservation, $\partial_t \rho + \nabla \cdot (\rho \, \mathbf{v}) = 0$, to obtain an equation that relates the variation in the pressure to the plasma displacement, $\underset{\cdot}{p} = (\gamma - 1) \, \boldsymbol{\xi} \cdot \nabla p - \gamma \nabla \cdot (p \, \boldsymbol{\xi})$. Variations in the magnetic field are related to $\boldsymbol{\xi}$ by Faraday's law, $\partial_t \mathbf{B} = \nabla \times \mathbf{E}$, and the ideal Ohm's law, $\mathbf{E} + \mathbf{v} \times \mathbf{B} = 0$, where $\mathbf{E}$ is the electric field, and we write $\underset{\cdot}{\mathbf{B}} = \nabla \times (\boldsymbol{\xi} \times \mathbf{B})$. The first variation in the energy functional resulting from arbitrary plasma displacements (and ideal constraints imposed on the variation of the pressure and magnetic field) is

$$\delta W = \int_{\mathcal{V}} (\nabla p - \mathbf{j} \times \mathbf{B}) \cdot \boldsymbol{\xi} \, dv - \int_{\partial \mathcal{V}} (p + B^2/2) \, \boldsymbol{\xi} \cdot d\mathbf{s}. \tag{5}$$

Ideal force balance is given by the venerated equation

$$\nabla p = \mathbf{j} \times \mathbf{B}. \tag{6}$$

This, the most important equation in the study of magnetically confined plasmas, simply states that plasma pressure gradients must be balanced by the Lorentz force.

### E. topology of the magnetic field

Ideal variations do not allow the "topology" of the magnetic field to change because of the frozen-flux condition [Fre87]. The word topology is enclosed in quotations because the word is not quite being used with the strict meaning used in the mathematical community. The word topology will hereafter describe whether the magnetic fieldlines lie on nested flux surfaces or whether the fieldlines are "irregular". (It is widely presumed that irregular fieldlines ergodically cover a non-zero volume, suggested [Meiss] to be the closure of the unstable manifold.) A magnetic field with nested flux surfaces is called "integrable" by an analogy with Hamiltonian dynamical systems, as will be described below.

The following theoretical and numerical models of three-dimensional (3D) equilibria may be classified by whether they apriori make assumptions regarding the topology of the magnetic field, usually enforced by constraining the numerical representation of the magnetic field, or whether the topology of the magnetic field is allowed to change *during* the equilibrium calculation.

### F. BETA, BETA-S & NSTAB

In the mid 1970s, Betancourt, Garabedian *et al.* developed the BETA code [BG75, BBG78, BBG82, BBG84], which assumed the magnetic field was integrable. The original version of BETA employed finite-differences in the radial, poloidal and toroidal coordinates.

Following the success of VMEC [HW83], BETA was converted to employ Fourier harmonics in the angles and was renamed BETA-S [Bet88]. This line of numerical work survives as NSTAB [Tay94].

Garabedian made every effort [Gar98, GM09, GM10] to explain that these codes use a "conservative discretization", and that this ensures that the numerical discretization captures the properties of the true solution in a mathematical "weak" sense.

Garabedian [Gar98] writes the partial differential equations of magnetostatics in the conservation form

$$\nabla \cdot \mathbf{B} = 0, \quad \nabla \cdot \mathbf{T} = 0 \tag{7}$$

where $\mathbf{T}$ is the Maxwell stress tensor given by

$$T_{jk} = B_j B_k - \delta_{jk} \left( p + \frac{B^2}{2} \right). \tag{8}$$

To avoid assuming the existence of partial derivatives, the divergence theorem is applied and $B$ and $p$ define a weak solution whenever

$$\int\int\int \sum B_k \frac{\partial \psi}{\partial x_k} dx_1 dx_2 dx_3 = 0, \tag{9}$$

$$\int\int\int \sum\sum T_{jk} \frac{\partial \psi}{\partial x_k} dx_1 dx_2 dx_3 = 0, \tag{10}$$

over any volume of integration, where $\psi_1$ etc. are arbitrary, continuously differential functions of compact support.

Because of this, Garabedian claimed [Gar98, GM09, GM10] that BETA-S, NSTAB *can* detect the formation of islands via a resonant deformation of the flux surfaces, even though the numerical discretization precludes the formation of islands. Convincing proof of this is shown in Fig. 1. When the resonant deformation is large compared to the

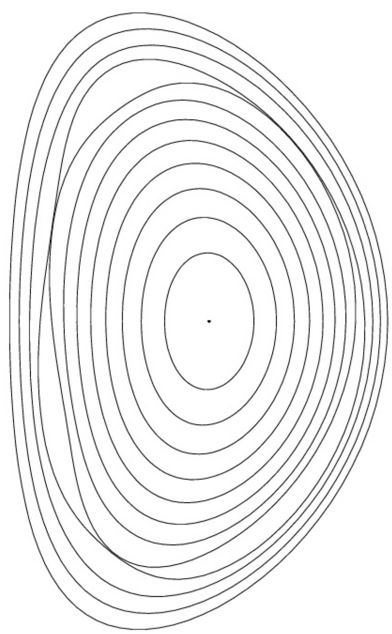

FIG. 1: Cross section of an unstable tokamak equilibrium displaying a magnetic island. From Garabedian & McFadden [GM10]

grid resolution, the numerical flux surfaces overlap and the code crashes.

(It would be interesting to place Garabedian's observations about the need for conservative discretizations that capture "shocks" and discontinuous solutions in context with Rosenbluth's [RDR73] observations that ideal MHD equilibria are not analytic functions of the boundary, with an understanding of how linear perturbation codes such as IPEC [PBG07] and CAS-3D [NB03] predict overlapping flux surfaces, and how these issues are resolved in ideal MHD if the rotational-transform is discontinuous across the rational surfaces [LHB+15], which implies the existence of sheet currents, which is exactly how Garabedian said islands would manifest themselves in equilibria with nested surfaces.)

It may be argued that it is *because* of the enhanced accuracy provided by the conservative discretization implemented in BETA-S/NSTAB, which yields the overlapping of flux surfaces, that BETA-S/NSTAB is less robust than VMEC, as is observed experientially. For practical reasons, the broader stellarator community prefers a robust code over a strictly mathematically rigorous code; and the global differences between NSTAB and VMEC are presumably/hopefully? small (for most cases of interest?). This was never quantified.

BETA-S was once used to study equilibria with islands [Bet88].

### G. Chodura & Schluter

In 1981, a method for extremizing the energy functional that *numerically* allowed for topological variations in the magnetic field was introduced by Chodura & Schluter [CS81]. The *theoretical* foundation of the algorithm, however, was based on ideal variations, which do not allow for topological variations. Any islands that did emerge could only arise from numerical "errors".

### H. SIESTA

(Skipping ahead chronologically . . . ) An approach similar to Chodura-Schulter has recently, in 2011, been revisited by Hirshman, Sanchez *et al.* in the SIESTA code [HSC11]. In SIESTA, a small amount of resistivity is initially introduced into the iterative scheme, and this allows the resonant flux surfaces to break into islands. The "intuitive interpretation" is that this resolves the problematic singularities in the parallel currents (singular currents are described in Sec. III K). Then, ideal variations are used to minimize the energy functional under the constraint of conserved topology, where the topology is generally a mix of flux surfaces, islands and chaotic fieldlines. The user may include some additional "resistive-iterations" as required to eliminate singularities; and the numerical scheme has incorporated methods for inverting singular and near-singular matrices (by shifting eigenvalues).

SIESTA is under active development: a free-boundary version was recently implemented [PRRBS$^+$17] and SIESTA has been used for equilibrium reconstruction [reported at ISHW 2017, and I think that W7-X calculations have been performed].

### I. Energy principle with a hierarchy of invariants

In the early 1980s, Bhattacharjee, Dewar *et al.* [BD82, BW83] revisited the mathematical formalism for ideal-MHD; and a numerical code [BWD 8] was introduced in 1984. The Bhattacharjee & Dewar formalism allows for a hierarchy of smooth, global constraints to be imposed on the class of variations used to minimize the energy functional. (Additional comments from A.B *et al.* are welcome.)

The original work of Bhattacharjee & Dewar restricted attention to integrable fields. Ideas from this work would later influence the theoretical development of multi-region relaxed MHD (MRxMHD), see Sec. III P, in which a hierarchy of discrete, local constraints are imposed on the variations.

### J. VMEC

Also in the early 1980s, Hirshman *et al.* began development of the now widely used VMEC code [HW83, HL86, HH86, HvRM86]. VMEC uses a representation of the magnetic field, $\mathbf{B} = \nabla\psi \times \nabla\theta - \nabla\chi(\psi) \times \nabla\zeta$, that assumes nested flux surfaces, where $\psi$ is the enclosed toroidal flux and $\chi$ is the poloidal flux, which is also called the magnetic fieldline Hamiltonian. The rotational-transform is $\iota\!\!\!-= d\chi/d\phi$. Given this representation for the magnetic field, the computational task is to find the geometry of the flux surfaces as defined by a coordinate transformation, $\mathbf{x}(\psi, \theta, \zeta)$. The toroidal angle is restricted to be the regular cylindrical angle, and the poloidal angle is adjusted [HM85, LHHN88, HB98] to minimize the spectral width of the coordinate transformation, which is effectively an adaptive grid in Fourier space and this provides numerical efficiency. (This was an important idea in 3D computations, and not just because of numerical efficiency). If the angle coordinates are not appropriately constrained, the solution in terms of the Fourier harmonics of the coordinate transformation is not unique, even though the geometry may be.) The derivatives of the energy functional with respect to the Fourier harmonics that describe the coordinate transformation are constructed, and an accelerated steepest descent algorithm is used to find minima of the energy.

The equilibrium is defined by the user-supplied pressure profile, and either the parallel current-density profile or the rotational-transform; and VMEC assumes that these input profiles are smooth and continuous. A finite-difference method in the radial direction is used [HSN90]. A preconditioner was implemented [HB91], and there are various extensions [Coo92, CHMG92].

VMEC is the fastest of the 3D codes, and is quite robust (too robust perhaps; see the above comments in Sec. III F). How accurately VMEC treats the rational surfaces has long been uncertain. Unlike NSTAB, VMEC shows no resonant deformation of the flux surfaces near low-order rationals, and VMEC allows for smooth pressure profiles with finite pressure-gradients across the rationals. (This is unphysical, see Sec. III K).

Most ideal linear stability codes, such as the global stability codes CAS3D [Sch93] and TERPSICHORE [?], infinite-$n$ ballooning codes such as COBRA [SHWW00], and transport codes, such as [?], assume the existence of nested flux surfaces. Many such codes have well-developed interfaces with VMEC.

VMEC presently forms the "engine" of existing stellarator optimization algorithms, e.g. STELLOPT [SHB$^+$01, LC13], and equilibrium reconstruction codes, e.g. V3FIT [HHK$^+$09] and STELLOPT [LC13]. V3FIT and STELLOPT are capable, in principle, of employing any (sufficiently fast) equilibrium code. However, stellarator optimization algorithms would be quite useless if one could not estimate the linear stability or transport properties; so appropriate stability and transport codes and appropriate interfaces will have to be developed if any code other than VMEC is to be used.

### K. singular current-densities, tangential discontinuities and infinite currents

The existence of pressure gradients *near* rational surfaces is unphysical. The perpendicular current-density consistent with ideal force balance is $\mathbf{j}_\perp = \mathbf{B} \times \nabla p / B^2$. By enforcing $\nabla \cdot \mathbf{j} = 0$, with $\mathbf{j} = j_\parallel \mathbf{B} + \mathbf{j}_\perp$, a magnetic differential equation then determines the parallel current, $\mathbf{B} \cdot \nabla j_\parallel = -\nabla \cdot \mathbf{j}_\perp$. Magnetic differential equations are densely singular, and thus are intractable numerically (see Sec. IV E for more discussion). For integrable fields the singular nature is exposed using straight fieldline coordinates, $\mathbf{x}(\psi, \theta, \zeta)$, and the magnetic field can be written $\mathbf{B} = \nabla\psi \times \nabla\theta + \iota\!\!\!-(\psi)\nabla\zeta \times \nabla\psi$. The Fourier harmonics of $j_\parallel$ must satisfy [BHH+95]

$$j_{\parallel,m,n} = \frac{i(\sqrt{g}\nabla \cdot \mathbf{j}_\perp)_{m,n}}{x} + \Delta_{m,n}(x), \tag{11}$$

where $\Delta_{m,n}$ is an as-yet undetermined constant and $x(\psi) \equiv m\iota\!\!\!-(\psi) - n$. The Jacobian satisfies $1/\sqrt{g} = \mathbf{B} \cdot \nabla\zeta$.

The $\delta$-function current-density is just a mathematical approximation of localized currents, and is acceptable in a macroscopic, perfectly conducting ideal-MHD model. (For example, the current-*density* associated with a finite current passing along a very thin strand of super-conducting wire is extremely well-approximated by a $\delta$-function.) Including $\delta$-functions in the current-density will result in a discontinuous magnetic field, and the magnitude of the $\delta$-function currents consistent with a given boundary and profiles can only be determined as part of a self-consistent equilibrium calculation.

The $1/x$ type singularity in Eqn. 11 is far more problematic. For a special choice of straight fieldline angles, namely Boozer coordinates [Boo82, DHCS91], the magnetic field may be written $\mathbf{B} = \beta(\psi, \theta, \psi)\nabla\psi + I(\psi)\nabla\theta + G(\psi)\nabla\zeta$, so that $1/B^2 = \sqrt{g}/(G + \iota\!\!\!- I)$, and

$$(\sqrt{g}\nabla \cdot \mathbf{j}_\perp)_{m,n} = \frac{p' \sqrt{g}_{m,n}(nI - mG)}{G + \iota\!\!\!- I}. \tag{12}$$

The magnitude of $\sqrt{g}_{m,n}$ may be considered to be an "output" quantity: it is determined by the geometry of, and the tangential magnetic field on, the rational surfaces, both of which are determined by the equilibrium magnetic field. For an arbitrary boundary, there is no apparent *a priori* control over the geometry of the internal flux surfaces. (The conditions for constructing "healed" equilibria are mentioned in Sec. VI G.)

Assuming the pressure satisfies $p(x) \approx p + p'x + p''x^2/2 + \dots$, the current through a cross-sectional surface bounded by $x = \epsilon$ and $x = \delta$, and $\theta = 0$ and $\theta = \pi/m$, associated with the resonant harmonic of the parallel current-density described by Eqn. 11 is

$$-\frac{2}{m} \frac{i(nI - mG)}{(G + \iota\!\!\!- I)} \frac{p' \sqrt{g}_{m,n}}{\iota\!\!\!-'} (\ln\delta - \ln\epsilon), \tag{13}$$

where all terms are evaluated at the rational surface. This approaches infinity as $\epsilon$ approaches zero.

This shows that there are cross-sectional surfaces close to every rational surface through which the total current is infinite, and this is unphysical. To guarantee such problems are avoided, and assuming that there are no restrictions on $\sqrt{g}_{m,n}$, the pressure-gradient must be zero on each rational surface. The next order term for the current through the cross-sectional surface is proportional to $p''(\epsilon)$, and so we must require that $p'' < \infty$. For any system with shear the rational surfaces densely fill space, and so either the pressure-profile is trivial, with $p' = 0$ everywhere, or the pressure-gradient must be discontinuous.

### L. what does VMEC compute at the rational surfaces?

However, examinations of the VMEC approximation to 3D equilibria reveal no such infinite currents, and the representation for the magnetic field does not accommodate discontinuities. We must conclude that VMEC is not exactly solving force-balance, $\nabla p = \mathbf{j} \times \mathbf{B}$, in the local vicinity of the rational surfaces, and that numerical resolution errors provide the required regularization of the singularities.

The most accurate investigation of how accurate the VMEC solutions are near the rational surfaces was recently performed by Lazerson *et al.* [LLHH16]. It was suggested that, because of finite radial resolution, that VMEC is effectively computing equilibria with discontinuous rotational-transform (see the stepped-transform equilibria mentioned in Sec. III S). Care must be taken when interpreting VMEC results, particularly when computing the linear stability of VMEC equilibria [GB92, MC93].

Despite the apparent theoretical flaws, it seems that VMEC is providing a reasonable *global* approximation to 3D MHD equilibria. In fact, experimental observations cannot distinguish between a variety of models [KSL+17]. As described by King *et al.* [KSL+17], DIII-D experiments using new detailed magnetic diagnostics show that both VMEC (nonlinear) and linear, ideal magnetohydrodynamics (MHD) theory quantitatively describes the magnetic structure (as measured externally) of three-dimensional (3D) equilibria resulting from applied fields with toroidal mode number $n = 1$. The comparison is shown in Fig. 2.

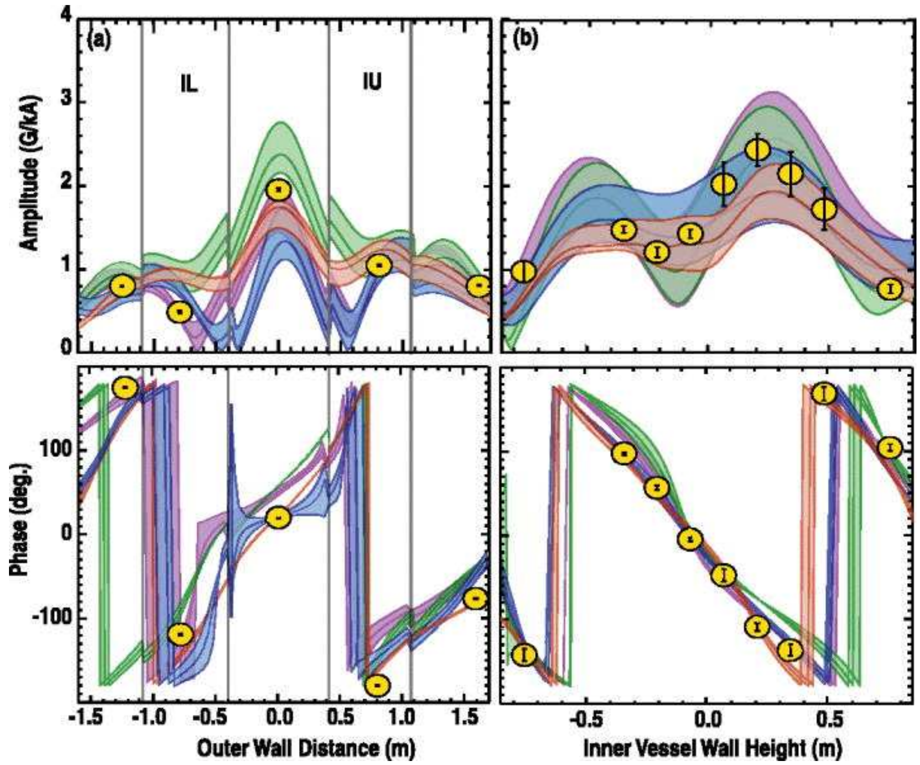


FIG. 2: The amplitude (top) and phase (bottom) of the poloidal field component of the $n = 1$ plasma response measured (circles with error bars) and calculated by the MARS-F (blue), M3D-C1 (purple), IPEC (green), and VMEC (red) codes along the (a) LFS at 5 vacuum vessel surfaces, including those containing the upper (IU) and lower (IL) I-coils and (b) HFS of DIII-D. Discharge 153485. From [KSL+17].

However, as also reported by King [KSL+17], at higher beta, near the ideal kink mode stability limit in the absence of a conducting wall, the qualitative features of the 3D structure are observed to vary in a way that is not captured by ideal MHD. (This might be evidence for the amplification of perturbations near stability limits in the stepped-transform mode Sec. III S as described by Loizu *et al.* [LHH+18].)

See also study by Reiman *et al.* [RFT+26].

### M. relaxed variations

Moving on to a different thread: in 1974, "relaxed states" were introduced by Taylor [Tay74, Rei81, Tay86]. These are states that minimize the energy functional allowing for globally *arbitrary* variations in the magnetic field that generally allow for reconnection; i.e., the topology of the field is not constrained. To avoid the trivial vacuum solutions, a constraint is included on the global helicity, so that the constrained energy functional becomes

$$\mathcal{F} \equiv W + \frac{\mu}{2}\left[\int_{\mathcal{V}} \mathbf{A}\cdot\mathbf{B}\, dv - H_0\right], \tag{14}$$

where $\mu$ is a Lagrange multiplier, and $H_0$ is the required value of the helicity. (There is also a constraint on the enclosed toroidal flux, and the boundary is constrained to be a flux surface.) The first variation in $\mathcal{F}$ resulting from arbitrary variations in the magnetic vector potential is

$$\delta\mathcal{F} = \int_{\mathcal{V}} (\nabla\times\mathbf{B} - \mu\mathbf{B})\cdot\delta\mathbf{A}\, dv. \tag{15}$$

The Euler-Lagrange equation shows that extrema have linear-force free fields, $\nabla\times\mathbf{B} = \mu\mathbf{B}$. Force-free fields have been considered in the 1950s by Chandrasekar & Kendall [CK13] and Woltjer [Wol58, Wol89]

### N. helicity

The helicity is a measure of the self-linkedness of the magnetic fieldlines [BF84, FA85, Ber99, Mof15], and intuitive understanding is that a weakly resistive plasma will rapidly evolve, perhaps turbulently, to minimize the plasma energy, but the plasma cannot so-quickly "untangle" itself.

Taylor relaxation can only be considered approximate. If the topology of the field is allowed to break because of resistivity, then the helicity is not strictly conserved. A recent paper by Qin *et al.* [QLLS12] discusses some recent ideas on this.

As it stands, there is not much about equilibria with pressure that simple Taylor relaxation can describe: Taylor relaxed states cannot accommodate pressure gradients.

With hindsight, given that both ideal and relaxed variations had been considered in context of extremizing the energy functional, it is perhaps not surprising that *mixed* ideal-relaxed equilibria would eventually be considered. This line of research would evolve from a a different thread, that of sharp-boundary states.

### O. sharp-boundary equilibria

In 1986, Berk, Freidberg *et al.* [BFL+86] introduced sharp boundary equilibria. This model was investigated in papers by Kaiser, Salat, Kress, Lortz, Spies *et al.* [KS94, LS94, Kai94, SL94, LS94, SLK01, Spi03, KU04]. In 1996, Bruno & Laurence [BL96] generalized from one relaxed volume to arbitrarily many, and allowed for pressure "jumps" between each volume. Theorems guaranteeing the existence of 3D equilibria with non-constant pressure were introduced, provided that the rotational-transform at the interfaces between each volume was sufficiently irrational. (The KAM theorem is invoked.)

It is the opinion of the author of this review (SRH) that this is when 3D MHD equilibria matured.

### P. multi-region relaxed MHD and SPEC

Multi-region relaxed MHD equilibria, introduced in 2006 by Dewar, Hole, Hudson *et al.* [HHD06, HHD07a, HHD07b, DHM+08, HMHD09, MHDvN10], are obtained by partitioning the volume into $N$ subregions, $\mathcal{R}_i$, separated by "ideal barriers". In each "relaxed volume", Taylor relaxation is assumed; and on each zero-volume ideal-barrier, the topological constraints of ideal MHD are enforced. The multi-volume constrained energy functional is

$$\mathcal{F} \equiv \sum_i \left\{ \int_{\mathcal{R}_i} \left( \frac{p}{\gamma - 1} + \frac{B^2}{2} \right) + \frac{\mu_i}{2} \int_{\mathcal{R}_i} \mathbf{A} \cdot \mathbf{B} \, dv \right\}, \tag{16}$$

where the required helicities in each region, the $H_0$'s, have been omitted for clarity. The Euler-Lagrange equations are equivalent to the stepped pressure states of Bruno & Laurence, namely that $\nabla \times \mathbf{B}_i = \mu_i \mathbf{B}_i$ in each relaxed volume and $[[p + B^2/2]] = 0$ across the ideal interfaces. The interface condition, $[[p + B^2/2]] = 0$, was recognized as a Hamiltonian system [BFL+86, BL96, MHDvN10], named the pressure-jump Hamiltonian. To satisfy the conditions for the KAM theorem for the pressure-jump Hamiltonian, the rotational-transform on the interfaces must be sufficiently irrational.

The stability of MRxMHD equilibria has been investigated in cylinder [MHD09] and theoretically in an honours thesis by Barmaz [Bar11]. Various theoretical extensions of the multi-region relaxed MHD (MRxMHD) energy principle have been considered: by taking the number of volumes, $N$, to infinity, MRxMHD reduces [DHDH13] to ideal MHD; flow [DHDH14b], pressure anisotropy [DHDH14a], and Hall effects [LAH16] have been introduced; and a Lagrangian variational formulation of multi-region relaxed MHD has been presented [DYBH15].

An enduring potential problem, however, is that the pressure and tangential magnetic field are discontinuous. Discontinuous functions are certainly not problematic for the equilibrium, as the energy principle is described by a volume integral, and the pressure and magnetic field in SPEC are certainly integrable (in the quadrature sense, not in the dynamical systems sense). However, discontinuous magnetic fields create problems for subsequent calculations of particle transport. Either SPEC needs to be reformulated so as to provide a continuous magnetic field (as described in Sec. III T), or the existing particle transport codes need to be modified to accommodate discontinuous magnetic fields.

In 2012, the Stepped Pressure Equilibrium Code (SPEC) code [HDD+12] was developed to construct MRxMHD states numerically. As an illustration, Fig. 3 shows a stepped-pressure equilibrium consistent with the boundary and profiles obtained via a 3D STELLOPT reconstruction [LLH+12] of an up-down symmetric DIIID experimental shot with applied resonant magnetic perturbation (RMP) fields. The pressure and $q$-profiles, where $q$ is the safety-factor $q \equiv 1/\iota\!\!\!{}^{-}$, derived from the reconstruction are shown as the smooth profiles. The stepped-pressure equilibrium consistent with the reconstructed boundary, a piecewise-flat approximation to the reconstructed pressure profile, and the reconstructed $q$-profile was constructed. The rotational transforms of the interfaces were chosen by selecting the most noble irrationals within range.

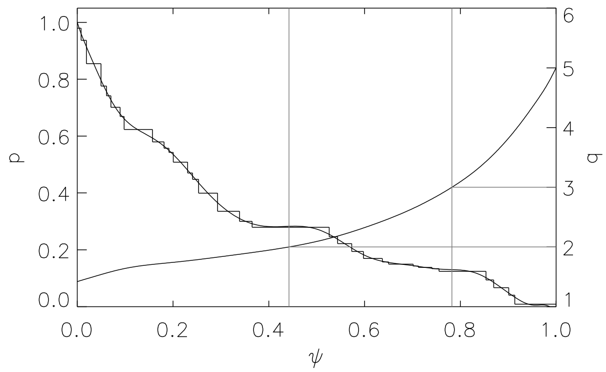


FIG. 3: Stepped pressure profile, from [HDD+12].

As the number of volumes approaches infinity, MRxMHD equilibria reduce to ideal MHD [DHDH13]. This allows SPEC to be used [LHBH15] to compute the singular current densities described in Sec. III K. SPEC has been verified against linearized calculations in cylindrical geometry [LHB+15], nonlinear calculations have been verified in stellarator geometry [LHN16], and predicted scalings of the Shafranov shift of the magnetic axis with pressure has been verified against analytic theory in a simple stellarator geometry [LHNG17]. SPEC is under active development: a publication describing free-boundary, non-stellarator-symmetric SPEC is presently under preparation, which includes a precise verification against a Biot-Savart code for vacuum fields.

SPEC has excellent convergence properties with respect to numerical resolution and all features of the stepped pressure states are resolved, including any singular currents that might be present, as these manifest themselves simply as tangential discontinuities in the magnetic field at the ideal interfaces. The primary motivation for developing SPEC was the work of Bruno & Laurence; and if theorems guaranteeing the existence of well-defined solutions can be developed, and if the numerical discretization accommodates the structure of the solution (i.e., if discontinuities in the magnetic field and pressure are allowed), then the numerical error should reliably and predictably decrease as the numerical resolution is increased.

### Q. free-boundary SPEC

A free-boundary capability has been implemented in SPEC and an article presenting a detail convergence study against a vacuum is under preparation [HLL18]. The energy principle is augmented to include a vacuum field,

$$W = \int_P \left( \frac{p}{\gamma - 1} + \frac{B^2}{2} \right) dv + \int_V \left( \frac{B^2}{2} \right) dv, \tag{17}$$

where $P$ is the plasma volume and $V$ is the vacuum volume. The inner boundary of the vacuum volume is coincident with the plasma boundary. The outer boundary of the vacuum volume, hereafter called the computational boundary is arbitrary, but a particularly convenient choice is to take this to coincide with the vacuum vessel. This has the advantage that singularities in the vacuum field produced by coil filaments are not present, and the magnetic field in the entire vacuum chamber can be computed as part of the equilibrium calculation. Transport across the edge of the plasma and head loads into the vacuum vessel can be computed.

The boundary conditions for the (total) magnetic field on the inner vacuum boundary $\equiv$ plasma boundary is $\mathbf{B} \cdot \mathbf{n} = 0$. On the outer boundary this is more complicated.

If the external coil geometries and currents are known and unchanging, then the magnetic field produced by the coils, $\mathbf{B}_C$, on the computational boundary can easily be calculated from Biot-Savart calculations. The complication arises because to provide the required boundary conditions to Laplace's equation, described in Sec. III B, we require the normal component of the *total* magnetic field, $\mathbf{B}_T \cdot \mathbf{n} = (\mathbf{B}_P + \mathbf{B}_C) \cdot \mathbf{n}$, but the magnetic field, $\mathbf{B}_P$, produced by the equilibrium plasma currents are apriori unknown.

A Picard iterative scheme has been tested and appears to provide an attractive algorithm [HLL18]. First, guess $\mathbf{B}_P \cdot \mathbf{n}$. If a better guess from a previous calculation is not available, choose $\mathbf{B}_P \cdot \mathbf{n} = -\mathbf{B}_C \cdot \mathbf{n}$, which will initially set the computational domain to be a flux surface. Using this, the free-boundary equilibrium calculation proceeds quite similarly to a fixed-boundary calculation; with the only difference is that there is an extra volume in which to compute the magnetic field (namely the vacuum volume) and the plasma boundary is allowed to vary until force balance is achieved, namely that $[[p + B^2/2]] = 0$. The computational boundary does not change.

After the free-boundary equilibrium has been constructed, we can now compute the magnetic field produced by the plasma currents (using the virtual casing principle [SZ72, Laz12, Han15]), and we can update the guess for $\mathbf{B}_P \cdot \mathbf{n}$

on the compuational boundary, and repeat. The Picard iteration is reliable because the dominant component of the total magnetic field on the computational boundary is provided by the external coils, which do not change during the free-boundary iteration. Note that the computational boundary will not generally be a flux surface, and a separatrix etc. can be accommodated in the vacuum domain.

This approach has been implemented [HLL18] in SPEC. A suitable coil set was provided by FOCUS . Shown in Fig. 4 is a verification calculation in a vacuum. The error between the SPEC field and the vacuum field approaches machine precision as the Fourier resolution in SPEC is increased.

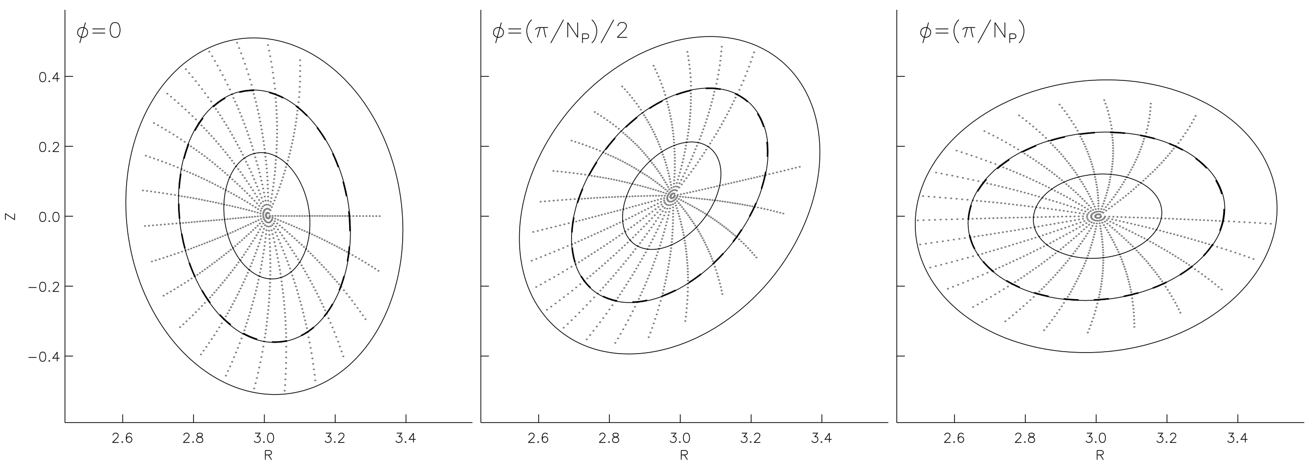


FIG. 4: A comparison between the Poincaré plots produced by using the magnetic field from a free-boundary SPEC "stellarator geometry" calculation and by using the magnetic field produced by the Biot-Savart law is shown. On this scale, the agreement is excellent. From [HLL18].

Note that the free-boundary approach described here only requires the vacuum magnetic field to be known on a two-dimensional surface, rather than on a three-dimensional volume (as is presently required for free-boundary VMEC). This will have computational advantages for a free-boundary optimization, for which the coil geometry is varied to obtain an optimal equilibrium.

### R. across the edge

The approach just described (in Sec. III Q) treats the region between the (smooth) plasma boundary and the vacuum vessel as being a vacuum. This a good place to start, but more realistic treatments are possible.

It is trivial in SPEC to treat this region as a force-free field (SPEC was designed compute force-free fields), and this would allow for plasma currents in the "vacuum" region.

Small pressure gradients may also play an important role. One approach for computing pressure gradients across the chaotic field is to employ the anisotropic diffusion equation,

$$\kappa_{\parallel} \nabla_{\parallel}^2 p + \kappa_{\perp} \nabla_{\perp}^2 p = S, \tag{18}$$

where $\nabla_{\parallel}$ and $\nabla_{\perp}$ are the parallel and perpendicular derivatives, and $\kappa_{\parallel} >> \kappa_{\perp}$ are the parallel and perpendicular diffusion coefficients. Nontrivial solutions can be obtained by setting the source, $S$, equal to zero, the pressure on the plasma boundary to be a constant, $p_{inn} = \epsilon$, and the pressure on the vacuum vessel equal to zero, $p_{out} = 0$.

This equation is computationally demanding as, in non-integrable fields, the length-scale of the solution is set by $\kappa_{\perp}$, and as $\kappa_{\perp}$ approaches zero the solution for the pressure becomes non-differentiable (i.e., a devil's staircase).

However, from nonlinear dynamics it is known that cantori play a crucially important role in restricting transport across ergodic fields, see Sec. V; and in appropriate coordinates, a remarkably simple expression may be derived. Chaotic coordinates [HB08] are constructed from piecing together the invariant structures of a nonintegrable field, namely the periodic orbits, KAM surfaces (if any) and the cantori, using so-called "ghost-surfaces". (Ghost surfaces are intimately related [HD09] to quadratic-flux minimizing surfaces [DHP94].) In such coordinates, an expression for the pressure gradient can be derived [Hud62],

$$\frac{dp}{ds} = \frac{const.}{\kappa_{\parallel} \varphi_2 + \kappa_{\perp} G} \tag{19}$$

where $s$ labels ghost-surfaces and their interpolates, $\varphi_2 \equiv \int B_n^2 ds$ is the quadratic-flux across the coordinate surfaces, and $G$ is a metric quantity. As $\kappa_{\perp} \rightarrow 0$, the pressure gradient becomes infinite on KAM surfaces, where $\varphi_2 = 0$.

Numerical methods for constructing chaotic coordinates have been described and implemented [HS90]. The construction of chaotic coordinates may thus be used to reduce what is demanding three-dimensional equation to almost trivially solved one-dimensional equations. To understand this, see Fig. 5, which shows how chaotic coordinates "untangle" the fractal structure of chaotic fields.

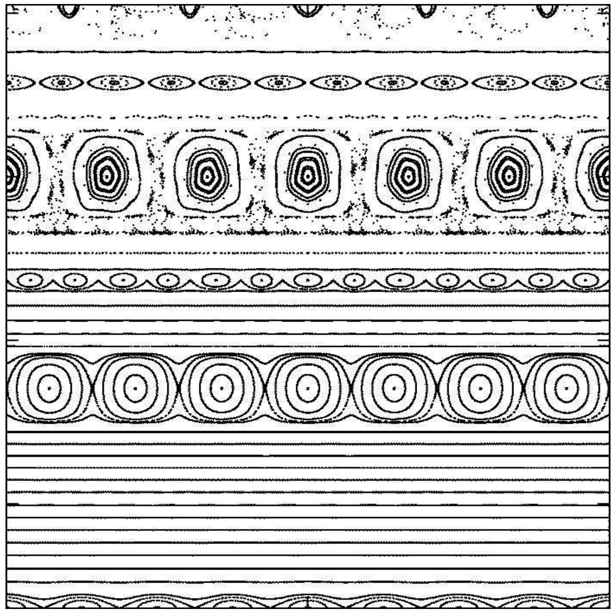

FIG. 5: Chaotic coordinates are coordinates adapted to the invariant structures of nonintegrable fields, namely the KAM surfaces, cantori and periodic orbits. Shown is a Poincaré plot for the LHD vacuum field across the plasma edge. The flux surfaces etc. become "flat", the islands become "square" and the pressure (as computed from the anisotropic diffusion equation) becomes a surface function. Reproduced from [HS90].

This (as yet) does not provide the self-consistent response that the small pressure gradients will have on the magnetic field. This might be treated using a suitable perturbation method. Other approaches have been considered for computing the 3D equilibrium in the presence of stochastic fields [RZM$^+$07, KR09, Rei00].

### S. stepped-transform, smooth-pressure equilibria

During the calculation of singular current-densities, it was realized that infinite shear was required to obtain tractable solutions. This was extended by Loizu, Hudson *et al.* [LHBH15, LHH$^+$18] to consider a class of 3D equilibria with nested flux surfaces, smooth pressure profiles and *discontinuous* rotational-transform profiles. Such equilibria avoid the singularities in the magnetic differential equations and the non-integrable current densities; and these equilibria are analytic functions of the boundary. In a sense, magnetic islands are modeled by sheet currents; as was known by Garabedian [Gar98].

This class of equilibrium gives qualitatively different results: external perturbations are not "shielded" by singular currents at the rational surface, and the perturbed displacement penetrates into the core, as shown in Fig. 6. .

### T. mixed ideal-relaxed MHD

An extension of multi-region relaxed MHD to include finite "ideal" volumes has recently been discussed [HK17]. Non-integrable current densities are avoided by allowing relaxation where the rotational-transform is rational. This model allows for smooth pressure and continuous magnetic fields. The *perpendicular* current-density is continuous, but the *parallel* current-density has discontinuities. The plasma volume is partitioned into alternating ideal and relaxed regions, and mixed ideal-relaxed energy functional is

$$\mathcal{F} \equiv \underbrace{\sum_{i\in\mathcal{I}} \int_{\mathcal{V}_i} \left(\frac{p}{\gamma-1} + \frac{B^2}{2}\right) dv}_{\delta\mathbf{B}=\nabla\times(\boldsymbol{\xi}\times\mathbf{B})} + \underbrace{\sum_{j\in\mathcal{J}} \int_{\mathcal{V}_j} \left(\frac{p}{\gamma-1} + \frac{B^2}{2}\right) dv}_{\int \mathbf{A}\cdot\mathbf{B}\, dv = H_j} . \tag{20}$$

In each ideal region, the topological constraints of ideal MHD are enforced; and to avoid the singularities in the parallel current the rotational-transform must be sufficiently irrational, e.g. $\mathbf{B} = \nabla\psi \times \nabla\theta - \iota\!\!\!{}^-_i \nabla\psi \times \nabla\zeta$, where $\iota\!\!\!{}^-_i$

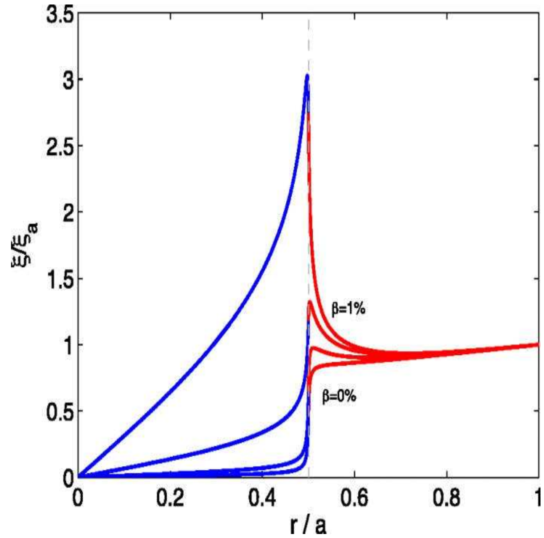


FIG. 6: Solutions of Newcomb equation for an $m = 2$, $n = 1$ boundary perturbation and for different values of $\beta$, from $\beta$=0 (lower curve) to $\beta$=1 (upper curve).

is a noble irrational. Smooth pressure profiles may be supported. With the pressure and rotational-transform being constrained, the parallel current is only known aposteori.

In each relaxed region, arbitrary variations in the magnetic field are allowed subject to the constraint of conserved helicity in each volume (i.e., Taylor relaxation). The pressure is flat, the parallel current is constant, and the rotational-transform is apriori unknown (in fact, if the magnetic reconnection leads to irregular magnetic fieldlines, the rotational-transform may be undefined). Example profiles for a 4-volume cylindrical example are shown in Fig. 7.

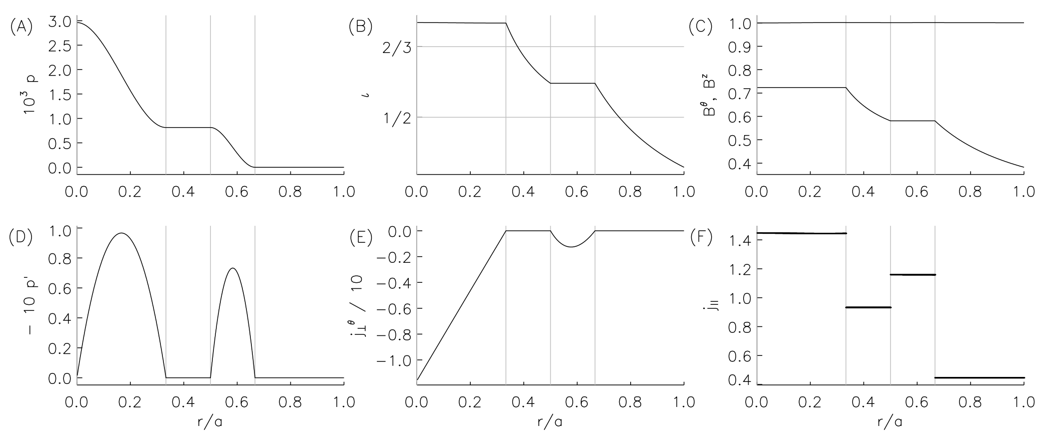


FIG. 7: An example, in cylindrical geometry, of a mixed ideal-relaxed equilibrium with 4 regions. A) The pressure profile. B) The rotational-transform profile. C) The "toroidal" and poloidal components of the magnetic field, $B^z$ and $B^\theta$. D) The pressure gradient. E) The poloidal component of the perpendicular current-density, $j_\perp^\theta$. F) The parallel current-density, $j_\parallel \equiv \mathbf{j} \cdot \mathbf{B}/B^2$. Reproduced from [HK17].

### U. explicitly fractal equilibria

Fractal equilibria with a Diophantine pressure profile and continuous magnetic fields have been constructed in cylindrical geometry [KH17]. The mixed ideal-relaxed energy principle [HK17] should allow fractal equilibria to be constructed in 3D geometry by taking suitable limits.

### V. non-linear "kink" states

Rosenbluth, Dagazian & Rutherford [RDR73], Boozer & Pomphrey [BP10], Loizu & Helander [LH17b],

### W. perturbed ideal MHD

Rosenbluth, Dagazian & Rutherford [RDR73] described how ideal equilibria are not analytic functions of the boundary, and that perturbation theory is not strictly valid.

However, it has been well demonstrated that linearized equilibrium codes such as IPEC [PBG07] and CAS3D-PEC [NB03] are useful experimentally. An intuitive reconciliation of this that even though the linearized codes predict a pathological response (the perturbed flux surfaces overlap), they give useful information about the sensitivity of an ideal plasma to particular distributions of error fields that either must be avoided or controlled.

## IV. RESISTIVE "INITIAL VALUE" CODES

### A. terminology

The terminology of 3D equilibria has historically been confusing. This review shall adopt the simple definition of an equilibrium code as an algorithm that computes the magnetic field consistent with a *given* pressure profile. A given current or rotational-transform profile is also required, and a given boundary or vacuum field is also required. An algorithm that allows the pressure profile to change during the calculation, and for the magnetic field to tear and islands/chaotic fieldline to form, will be called a resistive "initial value code". The definition is primarily required to distinguish codes that enforce topological constraints on the magnetic field and those that don't.

This definition of an initial value code includes codes that are "true" initial value codes, such as NIMROD [SGH$^+$03] and M3D-C$^1$ [JBF07], that faithfully integrate in time the equations of weakly resistive MHD to obtain a weakly resistive "steady state" and codes that use modified iterative schemes that seek to accelerate convergence to the desired solution.

### B. topological constraints of equilibrium codes

By the definitions just given, 3D equilibrium codes *must* enforce topological constraints. If the pressure profile is given, and the magnetic field that is consistent with the given pressure and with force balance, $\nabla p = \mathbf{j} \times \mathbf{B}$, is to be constructed, then because of $\mathbf{B} \cdot \nabla p = 0$ it is essential that flux surfaces coincide with pressure gradients. The condition $\mathbf{B} \cdot \nabla p = 0$ is effectively a topological constraint on the "output" of the equilibrium calculation, namely the magnetic field, imposed by the "input" pressure.

VMEC, NSTAB assume a smoothly nested set of flux surfaces, and thus they accommodate arbitrary smooth pressure and transform profiles. We may read this backwards: VMEC and NSTAB allow smooth pressure profiles, and so they must enforce smoothly nested flux surfaces. SPEC requires piecewise-flat pressure profiles, and so SPEC must enforce a *discrete* set of flux surfaces that coincide with the pressure jumps, where the rotational-transform must be irrational. SPEC enforces a much weaker set of topological constraints on the equilibrium than that of VMEC or NSTAB. The topological constraints imposed by SPEC manifest themselves as the ideal interfaces, and how many ideal interfaces are required is dictated by the input pressure profile.

The topological constraints enforced by SIESTA are somewhat mixed. During the relaxation iterations, the topology is unconstrained; but during the ideal iterations the topology is frozen-in to whatever topological state that was produced by the relaxation iterations, and this will generally be fractal. The amount of resistivity and relaxation introduced is at the user's discretion.

The codes described hereafter enforce no topological constraints on the magnetic field.

### C. resistive initial value codes

The simplest equations are an anisotropic diffusion equation for the pressure combined with the time evolution of the magnetic field and the velocity

$$\frac{\partial p}{\partial t} = \nabla \cdot \left( \kappa_{\parallel} \nabla_{\parallel} p + \kappa_{\perp} \nabla_{\perp} p \right) \tag{21}$$

$$\frac{\partial \mathbf{B}}{\partial t} = \nabla \times \left( \mathbf{v} \times \mathbf{B} - \eta \mathbf{j} \right) \tag{22}$$

$$\frac{\partial \mathbf{v}}{\partial t} = \tag{23}$$

If only the steady state solution, is required the algorithm can be accelerated by various adhoc modifications to accelerate convergence.

Early work by Park, Monticello *et al.* [PMWJ80];
HINT [HHS89, HST90, HMK+02]
Sugiyama with M3D [SPS+01]
Schlutt, Hegna *et al.* 's work [SH12, SHS+12, SHS+13] with NIMROD [SGH+03].

### D. Spitzer iterations and PIES

(This is not usually considered to be an initial value algorithm, but the pressure profile changes during the iterations and the topology is not constrained, and so it matches the definition of initial value code given in Sec. IV A.)

Spitzer [Spi83], Grad & Rubin [GR58] suggested the so-called iterative scheme. In 1986, Reiman, Greenside *et al.* [RG86, GRS89, RG90] implemented the iterative scheme in the PIES code. The iterative algorithm proceeds from an initial guess for the generally non-integrable magnetic field, $\mathbf{B}_n$, then updates the magnetic field and pressure according to:

$$\begin{aligned} \mathbf{B}_n \cdot \nabla p_{n+1} &= 0, & (24)\\ \mathbf{j}_{\perp,n+1} &= \mathbf{B}_n \times \nabla p_{n+1}/B_n^2, & (25)\\ \mathbf{B}_n \cdot \nabla \mathbf{j}_{\parallel,n+1} &= -\nabla \cdot \mathbf{j}_{\perp,n+1}, & (26)\\ \nabla \times \mathbf{B}_{n+1} &= \mathbf{j}_{n+1}. & (27) \end{aligned}$$

PIES was used in the fixed-boundary design of NCSX [HMR01]. A modification to the iterative scheme allowed a novel "coil-healing" algorithm [HMR+02]. This was achieved by splitting the total magnetic field into the part produced by the plasma and part produced by the external current-carrying coils, $\mathbf{B} = \mathbf{B}_C + \mathbf{B}_P$, and by including an extra equation that determined how the coil geometry should be altered at every iteration to eliminate the formation of magnetic fields, namely

$$(\mathbf{B}_{C,n+1} + \mathbf{B}_{P,n+1})^{\psi}_{m,n} = 0, \tag{28}$$

where $(\dots)^{\psi}_{m,n}$ denotes the resonant harmonic of the normal magnetic field at the resonant rational surface.

PIES developments include: initialization from VMEC [DMR05]; Newton method [ORM06]; application to W7-X [RZM+07].

### E. magnetic differential equations

To solve the magnetic differential equation for the parallel current-density in the iterative scheme, Boozer suggested using straight-fieldline magnetic coordinates [Boo84] constructed using fieldline following methods. Such coordinates diagonalize the linear operator appearing in Eqn. 26. Magnetic coordinates are analogous to action-angle variables, and action-angle coordinates cannot be constructed globally for non-integrable systems. Where the fieldlines are chaotic, the magnetic differential equation need not be solved in the iterative algorithm because the pressure is flattened by Eqn. 24, and the parallel current is constant in the volume covered by the ergodic fieldlines.

Several papers have considered the construction of magnetic differential equations [RG88, Rom89, RP91, LH92]. Hudson suggested a method that constructed straight fieldline coordinates on a set of pre-selected irrational surfaces [Hud04].

In order to allow pressure gradients in regions of chaotic fields, the iterative scheme was modified "resonance broadening" [KR09]

A regularized iterative scheme was suggested in [Hud10].

## V. DEVELOPMENTS IN CHAOS

To give a comprehensive review of non-linear dynamics would be overwhelming, but some understanding of chaos is required if we are to understand non-integrable magnetic fields and their effect on equilibrium and confinement.

The main points are (i) that there are well-defined structures in chaotic fields, such as the periodic orbits, cantori and KAM surfaces, the latter of which have a profound impact on transport across chaotic fields; (ii) that well-defined measures of chaotic transport (such as computing the flux across cantori) give important information regarding transport.; and (iii) that various numerical algorithms for reducing chaos have been successfully implemnted. The following is a quasi-chronological list of relevant publications.

The classical problem of small divisors . . . Action-angle coordinates cannot be constructed for non-integrable fields. There is a "small denominator" problem at resonances.

A theorem by Kolmogorov, Arnold and Moser (KAM) [Kol54, Mos62, Arn63] showed that, even though the perturbative transformation to action-angle coordinates cannot converge globally, it can converge locally if sufficient conditions are met, the most crucial is that the frequency (rotational-transform, $\iota\!\!\!-$) satisfies a Diophantine condition, $|\iota\!\!\!- - n/m| > d/m^k$ for all rationals $n/m$, where $d > 0$ and $k \geq 2$. Such irrationals are called "sufficiently" irrational. If the transformation to action-angle coordinates converges (elsewhere in this review these are called straight fieldline coordinates) then an invariant surface must exist, where "invariant" means that the surface does not change under the dynamical flow (i.e., the magnetic field is tangential to the surface). KAM proved that a finite measure of sufficiently irrational flux surfaces survive 3D perturbations. The importance of this mathematical theorem of Hamiltonian systems should not be under-estimated. If the KAM theorem were not true, we may not even have stellarators. (This amply illustrates that the fusion community relies on mathematical theorems; it is just that we don't know what all of the theorems are yet.)

It is easier to work with rationals rather than irrationals, and expressions estimating the size of magnetic islands given the perturbation are not too hard to derive. Chirikov [Chi79] suggested what is now a very widely used estimate: an irrational surface cannot exist if the nearby magnetic islands overlap. It is exactly the right idea, but is not very accurate, because of two problems. Large, low-order islands create smaller high-order islands, and it is the overlap of very small, high-order islands that destroys the invariant surfaces. Also, when things get too chaotic and separatrices split, it is not easy to determine the "size" of an island.

John Greene [Gre79, Mac92, MM83] provided a very insightful, precise method to determine the existence or otherwise of a given irrational surface (and it only really makes sense to describe an invariant surface by the rotational-transform). The existence of a given irrational surface is closely related to the stability of nearby periodic orbits. This is easily determined by the linear stability, as measured by the "residue". The other really good idea of Greene was to take the limit as $p/q \to \iota\!\!\!-$, where $p/q$ is the *best* rational approximation to a given irrational (to make sense of all this number theory see Niven [Niv56], who described continued fractions).

Percival [Per79b] suggested a variational principle whereby which irrational flux surfaces could be constructed.

A really important consideration, perhaps just as important as the KAM theorem, is that irrational surfaces never "die", but they rather gracefully "fade away". Percival, Aubry, Mather [Per79a, ALD83, Aub83, Mat82, Mat86] discovered the robustness of minimizers, i.e., that irrational fieldlines always exist.

It is easy to see how an irrational surface is traced out by an irrational fieldline. We need to be precise: in a finite "time", an irrational field*line* will never completely trace out an irrational *surface*, so what we really mean is the the *closure* of an irrational fieldline constitutes an irrational surface. The closure of a set is the set itself plus all the points that are arbitrarily close. An irrational surface is all the points that are traced out by an irrational fieldline plus all the points that the irrational fieldline comes arbitrarily close to after an infinite amount of time.

We know that invariant surfaces can be destroyed by island overlap, but the Aubry-Mather theorem shows that irrational fieldlines always exist. What gives? When an irrational surface is destroyed, the closure of an irrational fieldline ceases to constitute a surface; instead, it forms a cantor set, called by Percival a Cantor-torus, or cantorus for short.

Cantori have an extremely important effect on transport in stochasticity [MMP84a, MMP84b, MMP87, RKW91]. Any model of transport across chaos that ignores the effect of cantori, i.e. by assuming a random diffusion, is almost certain to fail for any magnetic field that is is fusion relevant. The diffusion model of transport is only relevant when the magnetic field is extraordinarily ergodic, and that means the plasma is lost almost immediately. We are, after all, trying to make the magnetic field as integrable as possible, and this is precisely when the diffusion approximation fails.

Non-integrable fields are a complex mix of Levy flights, the cantori are very "sticky" [Kar83, ECVD97], there is an infinite hierarchy of magnetic islands, the unstable manifolds associated with unstable periodic orbits . . . transport and exit times in chaos [BER94, Mei94].

To stand as "replacement" invariant surfaces when truly invariant flux surfaces have been destroyed, various definitions of "almost invariant" surfaces have been introduced, namely quadratic-flux minimizing curves [MD90, DM92] and ghost curves [Gol92, MM93].

Greene, MacKay *et al.* introduced methods to find the locally most robust irrational surface, the "boundary" circles [MS92a], which lie on the edge of chaotic regions (in plasma physics they are called last closed flux surfaces).

action-based variational methods

construction of cantori

Time reversal symmetry

### A. some mapping models

The standard map is most frequently used . . . see Greene [Gre79].

### B. from maps to flows

The magnetic field is a $1\frac{1}{2}$ dimensional Hamiltonian system, and the nonlinear dynamical theory of such Hamiltonian systems governs magnetic fieldline flow. This subsection describes some numerical methods that were originally developed for maps that have been applied to Hamiltonian flows.

Greene's residue was exploited to create vacuum magnetic fields with nested flux surfaces by Cary and Hanson. [Car82, HC84, CH86, Han94]. Later, Hudson and Dewar [HD97a] implemented a similar approach, which was extended to control not just the size but also the phase of magnetic islands [HD97b]. Cary and Hanson also provided an expression for the small island width [CH91]

Stellarator symmetry [DH98] was recognized as time reversal symmetry.

Ghost-circles were extended to ghost-surfaces, similarly for quadratic-flux minimizing curves [DHP94, HD96]. This was used to decompose a given field into an integrable field plus a small perturbation [HD98, HD99]

An extension of Percival's variational principle was applied to find irrational flux surfaces [Hud04].

Quadratic-flux minimizing surfaces were shown to be equivalent to ghost-surfaces [HD09, DHG12, DHG13].

Control of chaos by [CBC$^+$04]

Construction of cantori for fieldline flow [Hud06]

flux across islands, critical diagram

Ghost-surfaces [Hud07] were shown to be closely related to anisotropic diffusion [HB08, Hud62], and that chaotic-coordinates allows an analytic expression for the temperature gradient across an ergodic layer.

Chaotic coordinates were constructed for LHD [HS90].

Subtract from the total volume the volume of magnetic islands and we have the volume of flux surfaces. MacKay, Meiss have algorithms for quantifying the size of islands, and Cary & Hanson and others have applied similar ideas to creating integrable magnetic fields.

### C. numerical methods developed for flows

Computation of magnetic coordinates [RP91]. Construction of invariant tori and integrable Hamiltonians [KB94]

### D. island healing

Island healing methods [HD97a] were implemented for NCSX by Hudson *et al.* [HMR01, HMR$^+$02].

### E. diagnosing the structure of chaotic fields

Integrability means that everything is regular; ergodicity means that everything is random. Both admit useful theoretical approximations. Chaos means no simple approximation to anything is reliable. Any approach that makes simplistic assumptions about the structure of chaos is unreliable. Any numerical method that depends upon diagnosing the chaotic structure of phase space will be very slow, and very unreliable.

Any algorithm that seeks to accommodate non-integrable magnetic fields must accommodate the fractal structure of chaos. Using finite-differences on regular radial grids to resolve fractal structures will fail. As shown by Kraus and Hudson, fractal grids are needed to resolve fractals [KH17].

## VI. EQUILIBRIUM CONSIDERATIONS

What properties of the equilibrium do we desire? The task is not just to create an equilibrium state, we need an *attractive* equilibrium state. It is not really sufficient to just consider algorithms for the equilibrium calculation. The equilibrium theory is based on very simplified models, and equilibrium theory (by definition) cannot determine the transport. The transport determines the pressure profile, and the pressure profile determines the equilibrium magnetic field.

So, to understand what are the *relevant* equilibria, we must consider physics of magnetically confined plasmas that does fall under the category of equilibrium theory and numerics.

The following subsections describe i) what properties of the equilibrium magnetic field are required for confinement; and (ii) some non-equilibrium physics topics that have been shown to directly impact the equilibrium state.

### A. integrability

The principle of magnetically confined plasmas depends primarily on creating a “closed” magnetic field.

### B. rotational transform

To cancel out the electric field produced by particle drifts, the magnetic field must “twist” around the torus. This is called rotational-transform. Rotational-transform is necessary for magnetic confinement of plasmas, and the more the better.

What about shear? Perhaps low shear is good for near-integrability? Robert MacKay to explain . “My explanation is not so much that there are fewer rationals to consider, rather that averaging along the rationals that there are (or even could be if one changed a parameter) produces an exponentially better approximation to an integrable system when the shear is low, at least if the field is analytic.. . See [FC11].” and see a 1992 paper by MacKay (which one he didn’t say).

But what about instabilities? I thought that high shear breaks up instabilities and eddies . . . someone please discuss.

### C. Boozer coordinates

In the early 1980s, Boozer wrote a series [Boo81, Boo82, Boo83] of papers on 3D equilibria and a special class of magnetic coordinates that became known as Boozer coordinates.

### D. healed vacuum fields

“Healed” vacuum fields may be constructed by suitable manipulations of coil currents and/or coil geometries. Such techniques seek to reduce the size of low-order magnetic islands: Cary & Hanson [Car82, HC84, Car84, CH86]; and simple method to calculate island widths [CH91]; and also a method by Hudson & Dewar [HD97a, HD97b] that controls the phase of vacuum magnetic islands; and also control of chaos by [CBC+04].

### E. pressure induced self-healing

Pressure induced islands Cary & Kotschenreuther [CK85]; extended by Hegna, Bhattacharjee *et al.* [HB89, HBNW91]

Pressure-induced self-healing HINT calculations [HSM+94, GLHH97, LGHH98].

### F. finite-pressure island healing

Careful choice of the shape of the plasma boundary [HMR01] or coil geometry can produce finite pressure equilibria with [HMR+02] negligibly small islands.

### G. restricting attention to healed equilibria

Given that equilibria with nested surfaces are much more attractive for confining plasmas, the suggestion that equilibria can be “healed by design” suggest that that we can restrict attention to healed states, such as suggested by Weitzner [Wei14, Wei16], and the geometrical constraints on the equilibrium have been investigated. Intuitively, rather than considering the general class of 3D equilibria, it might be most practically relevant for the “equilibrium problem” to restrict attention to “healed states”, if and only if this can be ensured by suitable “design”.

### H. flow healing of islands

Hegna showed that plasma flow is important [Heg11] and can heal islands.

### I. equilibrium $\beta$ limits

[NWHB90], [Gar96], [LHNG17]

### J. importance of quasi-symmetry

Quasi-symmetry: [GB91];

### K. reducing turbulent transform

segwey into optimization . . . what is it that we want an equilibrium calculation for?

There is a fantastic amount of work on how flows heal islands, how quasi-symmetry reduces transport, how geometrical shaping can reduce turbulence . . . this section under construction . . . . Please provide relevant references . . .

[LMP$^+$09]

## VII. STELLARATOR OPTIMIZATION, COIL DESIGN AND REACTOR DESIGN

### A. knotatrons

Knotatrons [HSF44]! Kneed I say more?

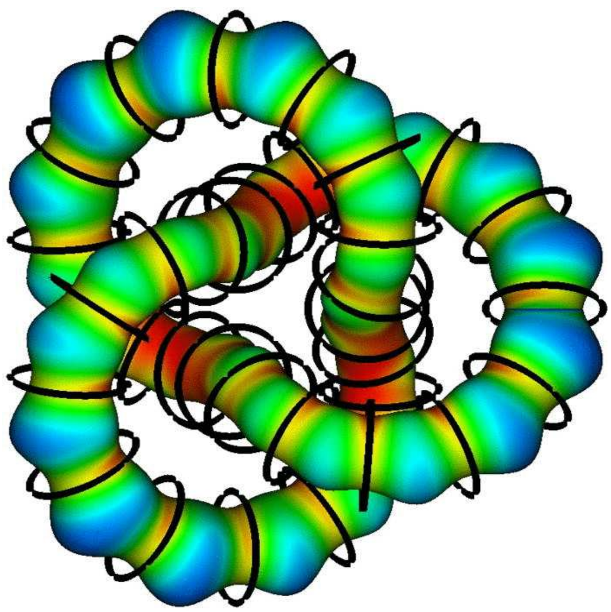

FIG. 8: Knotatrons, from [HSF44]

### B. coil design algorithms

There are two approaches that provide good starting points. The historical approach (NESCOIL [Merdf]) is to introduce a two-dimensional "winding" surface exterior to the plasma on which a continuous current distribution is assumed. The discrete coils are obtained as contours of the current distribution, which may undergo a further optimization (COILOPT), for example to reduce "ripple" created by discretizing the current potential. Landreman (REGCOIL[Land4]) has regularized the NESCOIL method; Landreman and Boozer have discussed which normal distributions of field are "efficiently produced", [LB16]. The optimal winding surface, however, is not known apriori, though there are some engineering constraints that influence how far from the plasma the coils can be (to allow access, blankets, . . .). Generally, methods that apriori require a winding surface need to perform a search for the optimal winding surface.

A recently suggested, more-direct approach is to start with a discrete representation of the coil geometry (FOCUS, [ZHSW0a]), and the magnetic field is provided by Biot-Savart given the geometry of a set of coils. To improve the efficiency of the numerical optimization, FOCUS has implemented the first and second derivatives [ZHSW18, ZHL+18] of how the magnetic field changes with respect to variations in the geometry, and this provides information about the sensitivity to coil placement errors.

### C. influence of plasma shape on coil cost

ARIES-CS reactor study: plasma coil separation [EGWH+08] Shape of the plasma determines the shape of the coils [LB16]

### D. existing stellarator optimizations

A lot of obviously relevant work has been performed on the topic of stellarator optimization [GLM+81, GBB+a0] and engineering design [BBG+15]. There is a huge amount of historical work on stellarators, restricting attention to "optimized stellarators", can include many papers on NCSX, W7-X optimization, ARIES-CS . . .

#### *1. NCSX optimization*

Zarnstorff [ZBB+00]; Neilson [NRZ+00]; Reiman [RKM+01]; Zarnstorff [ZBB+01];

#### *2. flexibility*

there was a dedicated issue of [Fusion Sci. Tech. **51**(2), 2007] describing NCSX design related research, including flexibility and robustness calculations [PBB+07];

#### *3. discharge evolution*

simulating the evolution of a discharge for NCSX [EL04]; We start with a vacuum, and we spray a little gas. Then we heat the gas. Isn't it true that the vacuum fields in stellarators must provide reasonable confinement? (Sorry, I have no clue about experiments.) One of the topics addressed below will be to address how to go from a vacuum to a high-pressure plasma whilst avoiding anything untoward.

Garabedian [Gar02, GM10]

#### *4. engineering designs*

Detailed engineering designs for advanced stellarators have been drafted [BBG+15].

#### *5. W7-X optimization*

[KAS+18]

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